SCIENCE AND TECHNOLOGY FOR ENERGY AND NATIONAL SECURITY

CRF NEWS

COMBUSTION RESEARCH FACILITY

March/April 2006 • VOL. 28, NO. 2

Investigating thermal stratification in HCCI engines

Most automotive and diesel engine manufacturers are engaged in significant efforts to develop an alternative piston-engine combustion process, termed homogeneous charge compression ignition (HCCI). HCCI engines operate by way of a dilute, premixed charge that autoignites and burns volumetrically as a result of being compressed by the piston. This combustion process is attractive because it can provide high fuel economy (similar to that of a diesel engine) while producing ultralow NO_X and particulate emissions. However, there are several technical challenges that must be overcome before HCCI will be practical. CRF researchers John Dec, Magnus Sjöberg, and Wontae Hwang are working to provide a fundamental understanding of the in-cylinder processes required to address these challenges.

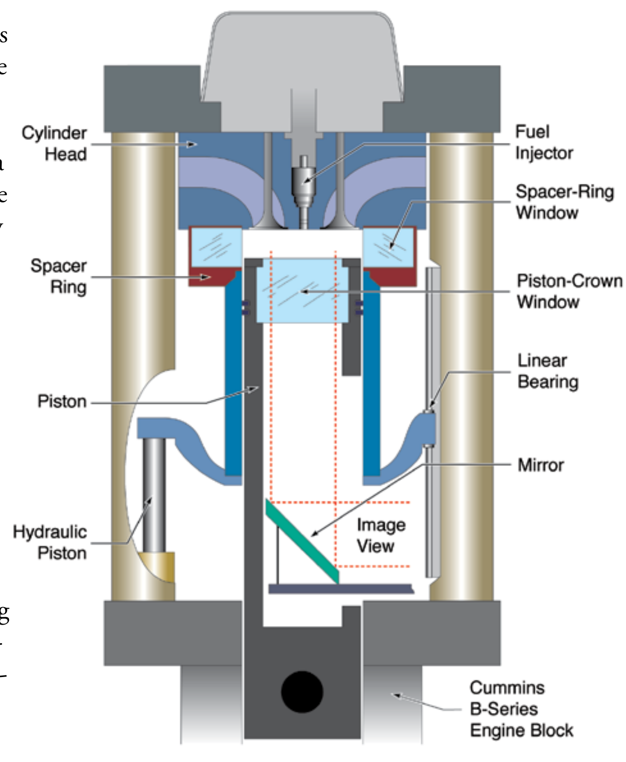

Figure 1. Schematic of the optically accessible HCCI research engine.

A key barrier to fully utilizing HCCI is that its power output is limited because the cylinder pressure-rise rate (PRR) resulting from the combustion process becomes too rapid. This overly-rapid PRR causes excessive noise and, eventually, engine damage. To understand the reasons for this limit and the potential for extending it, the team first compared the PRR in their research engine with that of a simulated engine with a fuel/air charge which was fully homogeneous in both mixture and temperature. (The Senkin application of CHEMKIN was used for this simulation.) The results showed that although the PRR in the real engine increased with the fueling rate, it remained well below what it would have been if the charge had been fully homogeneous. Thus, charge inhomogeneities in the real engine allow a higher power output than is feasible with a truly homogeneous charge. To investigate further, the team used an optically accessible HCCI research engine and image-intensified cameras to image at high speed the natural chemiluminescence light emission from the combustion process. As shown in Figure 1, this engine has an elongated piston that allows the combustion process to be imaged through the piston-crown window using a 45° mirror.

Typical piston-crown-window images, shown in Figure 2, confirm that HCCI combustion is not completely homogeneous, but has a distinct turbulent structure that changes as the combustion event progresses. To determine the cause of these inhomogeneities, Dec et al. conducted experiments at various operating conditions to change the potential sources of charge stratification. The results indicated that the primary source was

(Continued on page 2)

Coal ignition and devolatilization during oxy–fuel coal combustion with CO_2 recirculation

Capture of the carbon dioxide (CO_2) present in the exhaust gas of coal boilers, known as CO_2 sequestration, appears to be a feasible strategy to achieve zero-emission coal combustion. The process of sequestering CO_2 could be greatly facilitated if the gases leaving the boiler were composed of 100% CO_2. However, the conventional process of coal combustion in utility boilers uses air (79% N_2/ 21% O_2) to complete coal combustion. Combusting coal with air yields an exhaust stream containing N_2 as its main component (~75%), with a typical CO_2 concentration of 15% and the rest water (~7%) and excess oxygen (~3%). In contrast to coal combustion in air, coal combustion in pure oxygen produces a stream composed mainly of CO_2 (~70%) with a water concentration of ~27% with the balance as excess oxygen. After water condensation, the exhaust stream produced during coal combustion in oxygen would be basically CO_2, making sequestration a much more feasible technology than burning coal in air (see Figure 1, page 4). Unfortunately, coal combustion using100% oxygen would produce temperatures that damage the boiler components. To decrease flame temperature, it is necessary to dilute the oxidizing stream by recycling CO_2 into the boiler. This process of burning coal in oxygen with recycled CO_2 is known as oxy–fuel combustion with CO_2 recirculation.

The simplest O_2/CO_2 retrofit of air based coal boilers would be a direct substitution of the air stream by an O_2/CO_2 mixture. However, the different physical properties of CO_2 compared to N_2 cause differences in flame- and furnace operation parameters such as ignition time and gas-temperature profiles.

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Sandia National Laboratories

HCCI engines

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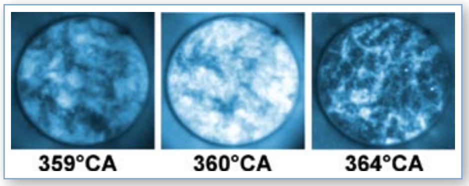

Figure 2. Typical chemiluminescence images acquired through the piston-crown window. The crank angle (CA) at the top dead center (TDC) of the intake stroke is given at the bottom (360°CA = TDC compression).

thermal inhomogeneities caused by heat transfer during the compression stroke combined with turbulent transport. Because of this thermal stratification, the entire charge does not autoignite simultaneously as it is compressed by the piston. Rather, combustion occurs sequentially as various regions reach their autoignition temperatures, as evident in the high-speed-movie sequence shown in Figure 3. This sequential autoignition slows the overall rate of combustion (and therefore the PRR), allowing considerably higher fueling rates than for a fully homogeneous charge.

This emerging understanding of how naturally occurring thermal stratification reduces the PRR suggests that attaining even higher loads could be achieved by enhancing this effect. But to determine the requirements of an ideal system, it is necessary to understand the required distribution of the thermal stratification.

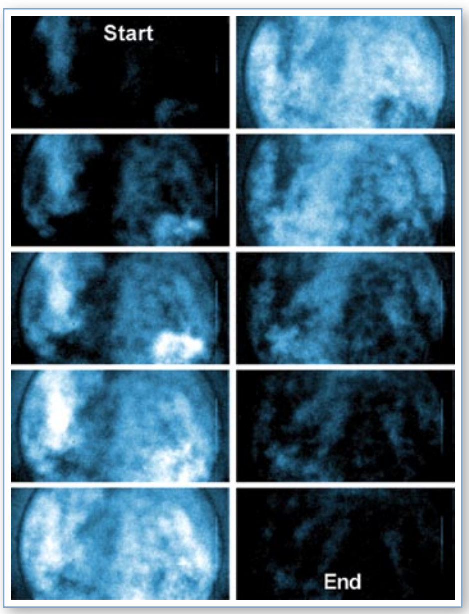

Figure 3. A high-speed movie sequence of chemiluminescence images obtained through the piston-crown window using a CMOS video camera. The interval between frames is 100 µs for the first five frames and 200 µs for the last five frames.

Since the heat transfer occurs at the in-cylinder surfaces, it is possible that thermal boundary layers play a major role in limiting the maximum PRR. To investigate this idea, Dec, Hwang, and Sjöberg imaged the combustion chamber from the side through one of the spacer-ring windows (see Figure 1) using a long depth-of-field lens to maintain image focus across the cylinder. Figure 4 shows a sequence of these images (each from a separate cycle) through the combustion event. The corresponding cylinder pressures, heat-release rates, and PRR are plotted in Figure 5. The images show that the early stages of autoignition at 360° crank angle (CA) produce a weak emission that is nearly uniform over the entire chamber. Then at 364° CA, hot ignition begins in localized regions near the vertical center of the combustion chamber. Over the next several CA degrees, additional regions in the central part of the charge autoignite and burn intensely, until the path-averaged side-view images appear nearly uniform in intensity. Eventually, this intense combustion in the central part of the charge begins to burn out, and the cooler boundary-layer regions along the cylinder head and piston-crown surfaces ignite and burn intensely (see the 372° CA image). However, this boundary layer combustion does not begin until well after the time of maximum PRR at 367.7° CA (see Figure 5). Thus, for thermal stratification to be effective in reducing the maximum PRR and allowing higher loads, it must be distributed throughout the bulk gases in the central part of the charge. Thermal stratification in the boundary layer has only a secondary effect.

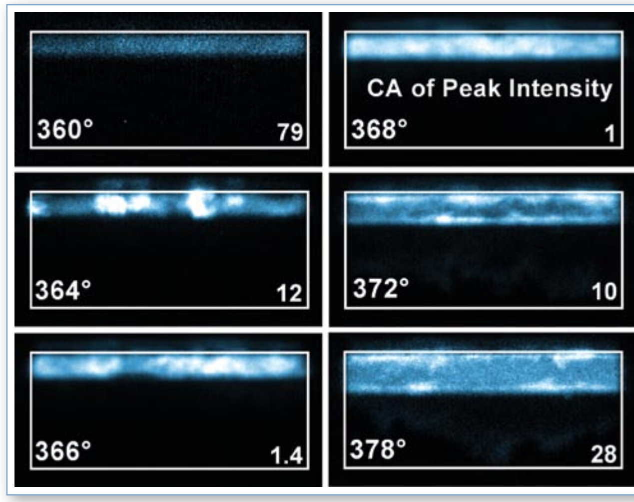

Figure 4. A sequence of images (each from a separate cycle) of the HCCI combustion acquired through a spacer-ring window. The relative intensifier gain is given at the lower right.

These results, combined with multizone kinetic modeling, show that if the bulk-gas thermal stratification could be increased even moderately, significantly higher loads could be reached. Future studies are planned to investigate various methods that could potentially achieve this.

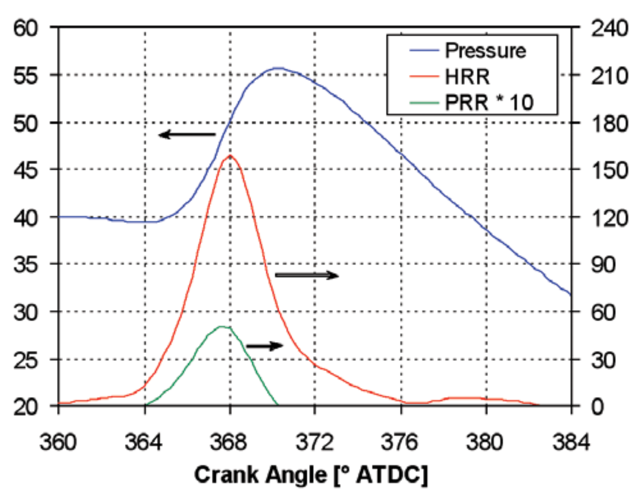

Figure 5. Cylinder pressures, heat-release rates and the PRR (derivative of the cylinder pressure) for conditions corresponding to those of the images in Figure 4.

The Eighth International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames (TNF8) will be held 3–5 August, 2006, in Heidelberg, Germany, just before the 31st Combustion Symposium. The TNF Workshop series, coordinated by Rob Barlow, is an open and ongoing international collaboration among experimental and computational researchers in turbulent combustion. Further information is available at *http://www.ca.sandia.gov/TNF.*

Engines group hosts ACC-HCCI working group

This spring, Engine Combustion Research hosted the Advanced Engine Combustion/Homogeneous Charge Compression Ignition working group meetings, which focus on the in-cylinder processes governing gasoline and diesel combustion. Following the AEC meetings were presentations of research in HCCI or Low Temperature Combustion performed at the University of Wisconsin, the University of Michigan, Massachusetts Institute of Technology and Stanford University under contract to the Department of Energy. Working group members include Cummins, General Motors, Caterpillar, Inc, Detroit Diesel, Ford, Daimler Chrysler AG, John Deere, International Truck, and Mac Trucks, as well as research institutions Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Argonne National Laboratory, and Oak Ridge National Laboratory.

Uen Do Lee (right) is a visiting researcher this year from the Combustion Engineering Research Center (CERC) of the Korea Advanced Institute of Science and Technology (KAIST). Working with Jonathan Frank and Sebastian Kaiser, Lee is studying how unsteady flows affect ignition of hydrocarbon fuels in a counterflow configuration.

Postdoc Richard (Renfeng) Cao (left) will join the Shell Unconventional Resources group in Houston, TX in early April to work on the in-situ conversion process of oil shale. At the CRF, Cao worked with Habib Najm, focusing on the modeling and computation of low-Mach-number reacting flows.

Fiber laser grand challenge

The Fiber Laser Grand Challenge, a project funded by Sandia National Laboratories' Laboratory Directed Research and Development (LDRD) office, held its third External Advisory Board review on February 9, 2006. Board members include William Schneider (Chair, Defense Science Board), William Thompson (Air Force Research Laboratory), Michael Dennis (Johns Hopkins Applied Physics Laboratory), and Randy Bell (NNSA). In its report, the board stated that it "...is unanimous in its opinion that the Fiber Laser Grand Challenge team has made excellent progress toward its technical objectives.... The team has consistently metand exceeded its technical objectives (often well ahead of schedule), and has adjusted its priorities to focus on the most important tasks while taking advantage of external advances." The project is now half way through its 3-year duration.

Jean-Philippe Feve

Jean-Philippe Feve (right) of Teem Photonics visited the CRF fiber-laser laboratory for a week in February to conduct proof-of-concept experiments on a new laser system with Roger Farrow (left), Paul Schrader, and Dahv Kliner. Using a prototype microchip laser developed by Teem and a Yb-doped fiber amplifier developed by Sandia, the team demonstrated broad tunability in repetition rate (from 4 to 28 kHz) while maintaining constant pulse duration (1.1 ns) and narrow spectral width in a compact, efficient system. Such a laser source will be useful for numerous applications, including remote sensing, materials processing, and nonlinear frequency conversion to generate wavelengths from the mid-IR through the deep-UV.

Dr. Seungmook Oh

Dr. Seungmook Oh, a long term visitor to the CRF from the Korea Institute of Mechanics and Machinery, is working with Paul Miles to investigate the in-cylinder distribution of unburned and partially-burned fuel.

Coal ignition and devolatilization (Continued from page 1)

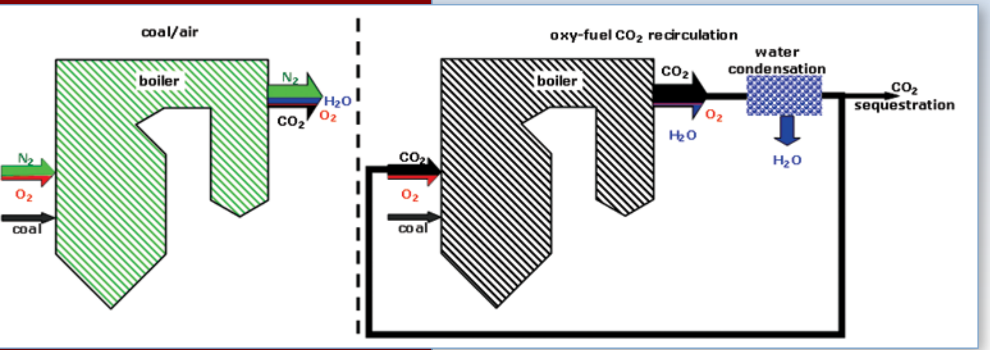

Figure 1. Comparison of coal/air and oxy–fuel with CO_2 recirculation schemes.

In experiments carried out in the optical entrained-flow reactor at Sandia National Laboratories, Alejandro Molina and Chris Shaddix measured the variation of ignition and devolatilization times for ~ 100µm-diameter particles of a typical type of eastern U.S. bituminous coal, under combinations of O_2/CO_2 and O_2/N_2 comparable to those used in coal utility boilers.

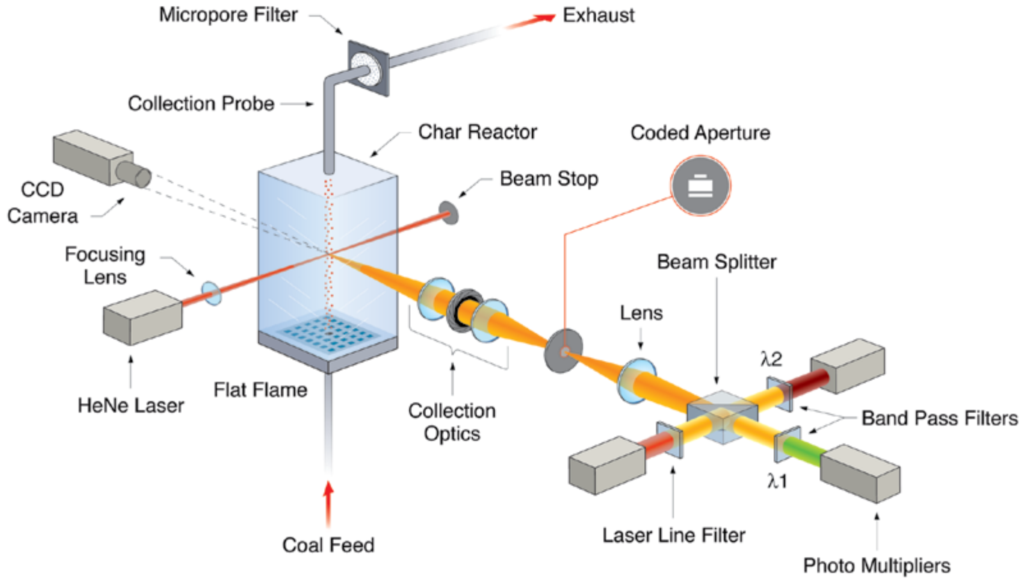

Figure 2. Entrained flow reactor and associated optical diagnosis.

Figure 2 shows a schematic of the facility. The burner operates at one atmosphere and uses a diffusion flamelet-based Hencken burner. Solid fuel particles are injected at the furnace centerline. A quartz chimney isolates the reacting particles' burner products from the surrounding air so optical measurements can be performed on the particles injected into the flow. The effect of the presence of CO_2 on coal ignition was simulated by entraining coal into mixtures with N_2 or CO_2 as balance gas at three different oxygen concentrations at a temperature of 1700 K.

Images of individual burning coal particles were obtained by using a signal from a Helium Neon (HeNe) laser that triggered an ICCD camera when a particle entered the camera's focal point. A combination of bellows and focusing lenses focused the camera on small flying coal particles. Single-particle imaging showed that substituting N_2 with CO_2 increases the time required for ignition. It also demonstrated that the temperature and size of the diffusion flame of the soot cloud that surrounds the particle are lower and larger respectively, when CO_2 is used instead of N_2. The size of this cloud also decreases as the oxygen concentration increases, as Figure 3 shows. For homogeneous ignition, such as observed in the experiments, these effects can be explained by the higher density and heat capacity and lower diffusivity of CO_2 when compared to those of N_2. The changes in volatile flame behavior and ignition delay times in the presence of CO_2 observed for single particles should also be present in coal combustion in utility boilers. However, the results of this investigation suggest that an increased oxygen concentration for CO_2 recycle combustion, if correctly selected, could produce ignition times and volatile flames similar to those obtained under coal/air combustion.

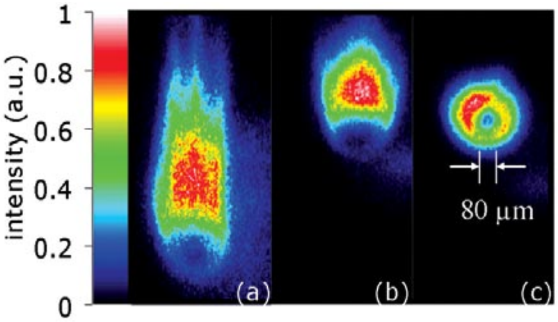

Figure 3. Examples of images of the soot-cloud surrounding coal particles in CO_2 for various oxygen concentrations: (a) 12% O_2, (b) 24% O_2, and (c) 36% O_2.

Edgar Estupinan

Postdoc Edgar Estupinan will be taking a R&D position at Osram Sylvania in Beverly, MA. Estupinan worked with Craig Taatjes studying the kinetics and mechanisms of alkyl radicals with O_2, as well as conducting validation experiments on theoretical models developed by Jim Miller and Stephen Klippenstein.

Feng Tao

Feng Tao, a postdoc in Professor David Foster's laboratory at the University of Wisconsin-Madison, visited the CRF from February to March 2006. Tao worked with Lyle Pickett and Andy Lutz on the soot modeling of diesel combustion.

Development of practical and efficient high-power lasers

Laser-based methods offer unique capabilities for a variety of applications, including ultrasensitive detection of trace species, chemical and physical sensing (remote and in situ), secure high-speed telecommunications, and materials processing. Although laser-based techniques show tremendous promise, many potential applications have been rendered impractical by the limitations of existing technology. Traditional high-power laser systems are large, heavy, power consumptive, inefficient, complicated, and unreliable. Rare-earth-doped fiber lasers and amplifiers are solving these problems, and fiber lasers are rapidly displacing conventional laser systems in a wide variety of applications. Furthermore, this innovative technology is enabling a number of new applications because of the following practical attributes: its compact size, light weight, high efficiency (low power consumption), ruggedness, reliability, facile thermal management, and diffraction-limited beam quality.

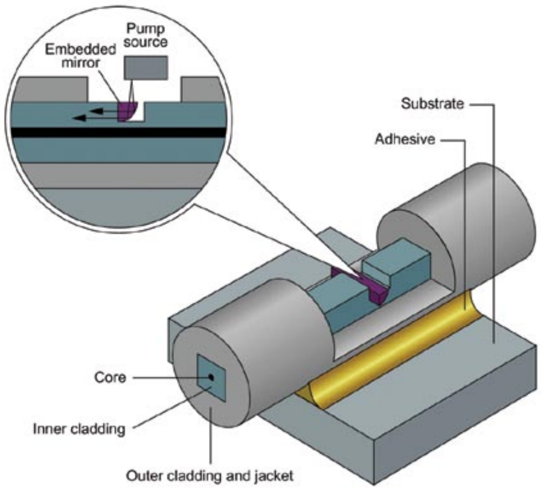

Figure 1. Schematic diagram of the EMSP hardware with the micro mirror shown in purple and the fiber core in black. The pump beam is launched into the inner cladding (blue).

In a fiber amplifier, the gain medium consists of a rare-earth ion (typically Yb^{3+} or Er^{3+}) doped into the core of an optical fiber. The rare-earth ions are pumped using a diode laser, which provides high optical power (>6-W from a 100-µm x 1-µm aperture) with high efficiency (>50% wallplug). A key challenge is to efficiently and stably launch the output from the pump diode into the gain fiber. Sandia researchers have developed a side-pumping method to accomplish this task (*CRF News* Vol. 24, No. 4). Recently, they demonstrated the use of this technique to directly launch the output of a diode bar, which is the most cost-effective, compact source of high pump power (presently >100-W per bar), with much higher efficiency and system simplicity than any competing method.

Embedded-mirror side pumping

Diode lasers are a nearly ideal pump source, but the output beam is highly divergent and astigmatic and is therefore poorly matched to the fiber (which is generally round and has a limited acceptance angle). The development of efficient, practical pumping methods is an active area of research. Jeff Koplow, Sean Moore, and Dahv Kliner of the Remote Sensing Group have developed a method, embedded-mirror side pumping (EMSP), in which a channel is polished into the side of the fiber, and a micromirror (~50-µm in diameter) is inserted into the channel (Figure 1). The pump diode is mounted in close proximity to the micromirror (~15-µm separation), and the diode output beam is launched into the fiber by reflection from the mirror. EMSP offers the following advantages:

- Efficient coupling (typically >85%)
- Low alignment sensitivity (and thus long-term stability)
- No loss for the signal beam propagating in the fiber core;
- No obstruction of the fiber ends
- Low parts count
- Compact and rugged packaging
- Compatibility with a variety of fiber types and pump sources
- Low cost

Furthermore, because the mirror is manufactured separately from the fiber, its properties can be independently designed and optimized. The current mirror design greatly reduces the divergence of the pump diode (thereby reformatting it for efficient coupling into the fiber), has a broad acceptance angle, and provides high reflectivity independent of the pump spectrum and polarization state. EMSP has been used to construct fiber amplifiers for a variety of applications, typically using one or two pump diodes per amplifier.

Further power scaling can be accomplished by mounting additional pump diodes along the fiber, but this approach increases the system's complexity and assembly time because each diode has to be separately aligned and mounted. It would be preferable to employ a diode bar, which is a monolithic linear array of diode lasers (typically 10–30 emitters evenly spaced along a 1-cm bar). Diode bars are by far the most cost-effective source of high pump power (<$25 per watt, a factor of 4 lower than single emitters), but the closely spaced array of astigmatic output beams is very poorly formatted for coupling into a fiber. As a result, existing methods employ bulk optics to reformat the diode-bar output and to launch the reformat-

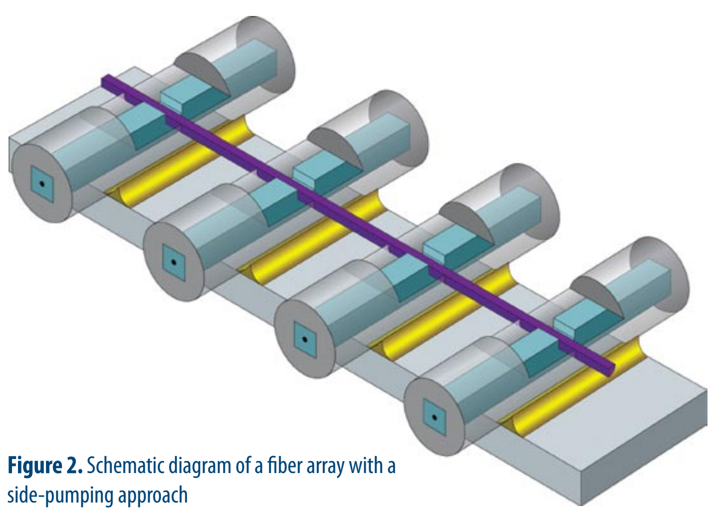

Figure 2. Schematic diagram of a fiber array with a side-pumping approach

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High-power lasers *(Continued from page 5)*

ted beam into a passive fiber, whose output is in turn coupled into the gain fiber. This method greatly increases the system's cost, size, and complexity, and it inevitably causes loss of power or efficiency (the typical net coupling efficiency is ~50%).

Direct diode-bar pumping

In contrast to conventional pumping methods, EMSP is capable of directly coupling the output from a diode bar into a fiber or fiber array, as shown in Figure 2. The gain fiber is mounted with successive pump-injection sites spaced with the pitch of the diode bar. The channel intersects the fiber at multiple points, and a single mirror is inserted across the channel. As in the case of a single emitter, the diode array is mounted in close proximity to the mirror. This approach is feasible because of the large alignment tolerances of EMSP.

Moore, Koplow, Kliner, and two students (Georg Wien and Andrea Hansen) recently performed the first proof-of-concept experiment demonstrating diode-bar EMSP using a 10-emitter (20-W) bar and a 10-fiber array. They obtained a net coupling efficiency of 85%. Compared to the conventional approach previously described, the wasted power was reduced by more than a factor of 3 (from ~50% to 15%), and the system complexity, size, and cost were vastly reduced (Figure 3 shows a photograph of the assembled hardware). In addition, the researchers showed that the coupling efficiency from a given emitter into its corresponding fiber was independent of whether the emitter–fiber pair was aligned separately or as part of the net system alignment, verifying that the performance was not degraded by scaling from one emitter to ten.

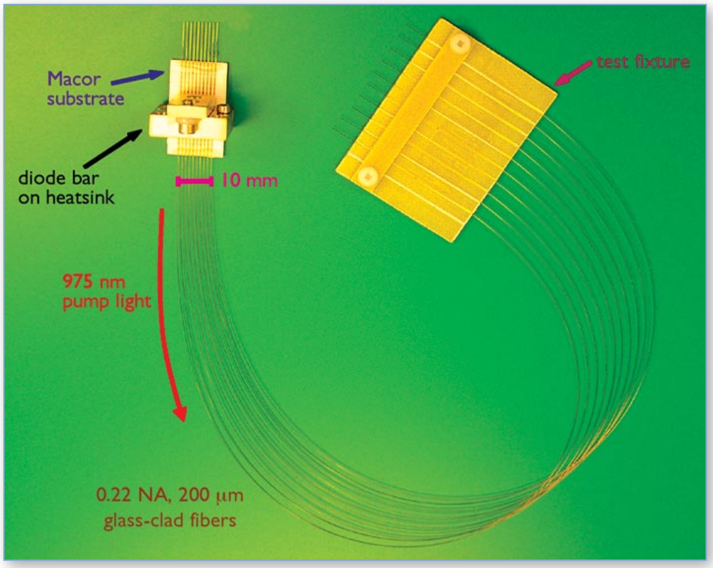

Figure 3. Photograph of the diode-bar-pumped fiber array employed in the proof of concept experiments.

Embedded-mirror side pumping is the only method capable of directly coupling the output of a diode bar into a gain fiber. This technique allows remarkably graceful power scaling because it does not increase the complexity, parts count, alignment sensitivity, or number of fabrication steps compared to pumping with a single emitter. These unprecedented characteristics will enable development of uniquely practical, economical, and efficient high-power lasers. The researchers are now constructing a Yb-doped fiber amplifier employing this method.

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CRF News is a bimonthly publication of the Combustion Research Facility, Sandia National Laboratories, Livermore, California, 94551-0969.
ISSN 1548-4300

Director .... Terry Michalske
Editor .... Wendy Wolfson
Graphic Artist .... Daniel Strong
Photography .... Daniel Strong/Various Photographers

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC0494AL85000